Benchmark of an efficient BGK model for rarefied gas flows in full 3D geometry

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Outline

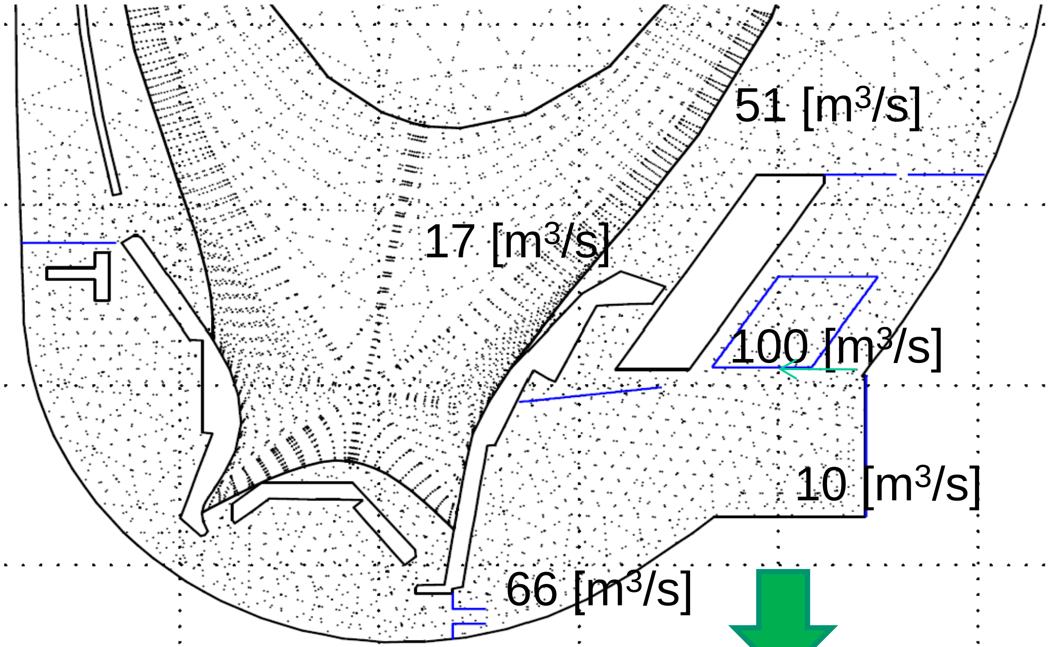
- Introduction:
    1. basic considerations on rarefied gas flow in fusion system and and related pumping
    2. conductances and flow regimes @ ASDEX Upgrade (AUG)

- Benchmark of EIRENE Monte-Carlo particles transport code (a standard in nuclear fusion) with ~ isothermal flows
    1. Numerical method using EIRENE
    2. Set up of numerical experiments
    3. Test cases:
        a) A channel length scan in free molecular regime
        b) Pressure scan for a slit and short channels
        c) Pressure scan for a orifice and pipes

- Prospective and conclusions

AUG conductance modelling: FMR

By-passes measurements



- The AUG poloidally and toroidally distributed ducts (3D) can be mimed in EIRENE with poloidally distributed (2D) (and toroidally uniform) ducts preserving the total effective conductance in free molecular regime

model	AUG ducts measurements	Best match EIRENE model
Main chamber to pump chamber	51 [m^3/s]	51 [m^3/s]
Divertor to pump chamber	17 [m^3/s]	17 [m^3/s]
Sub-divertor to pump chamber	66 [m^3/s]	50 [m^3/s]
Total	134 [m^3/s]	118 [m^3/s]

Divertor neutrals flow regimes

Range of K_n	Flow regime	Governig eq.	AUG regime
$K_n < 10^{-3}$	Fluid-continuum	Euler, Navier-Stokes	None
$10^{-3}<K_n<10^{-1}$	Slip	Navier-Stokes with slip flow	#25681, K_n=0.027
$10^{-1}< K_n<10$	Transition	Boltzmann	L-mode, H-mode $K_n \geq 0.1$
$10 < K_n$	Free molecular (FMR)	Boltzmann with no collision	Low density L-mode $K_n \leq 25$

- Not only future devices but even today's exp. (AUG, C-Mod) are often in transition regime!
- But EIRENE tested only for Couette flow …

EIRENE: Monte-Carlo transport code

Solves multi-species Boltzmann equation in BGK approximation for neutrals:

$$\frac{df_i}{dt} = \nu_i \left(f_M - f_i \right)$$

- Solution by „*successive linearisation*" [1]:
  - Test particle trajectories are simulated and from the test particle distribution, new moments are derived for the Maxwellian of the next iteration
  - Iterations are repeated until equilibrium is reached either by fixing upstream density of influx of particles

- Sampling the trajectories of the neutral particles (H, H2, He, C…) in a given background of plasma and neutral particles. Cartesian, triangular or tetrahedral grids. Designed specially for fusion applications (definition of sources, coupling to plasma codes etc.)

[1] Reiter D., May Ch., et. al, J. Nucl. Mater, **241-243, 342 (1997)**

Code features

- f_M is a drifting Maxwellian (equilibrium solution), depending on local moments of in order to ensure particle, momentum and energy conservation

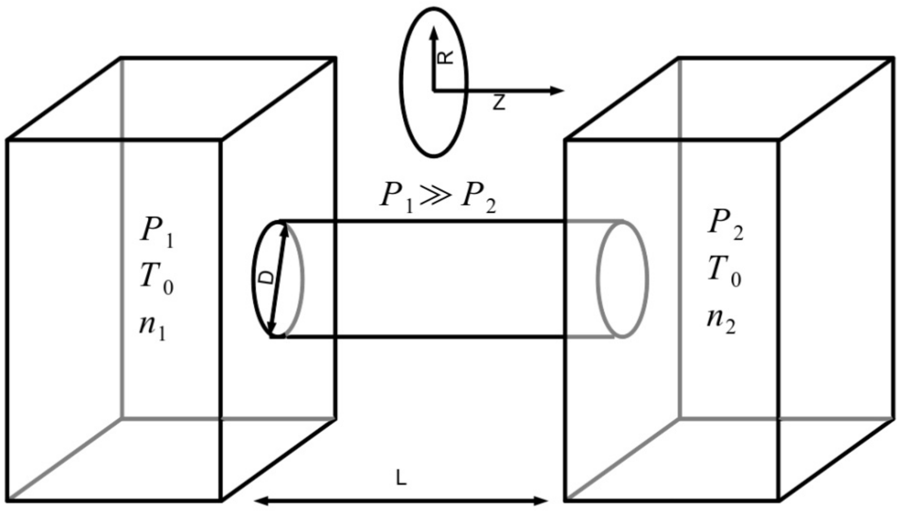
- ν_i are a collision rates deduced from experimental viscosity

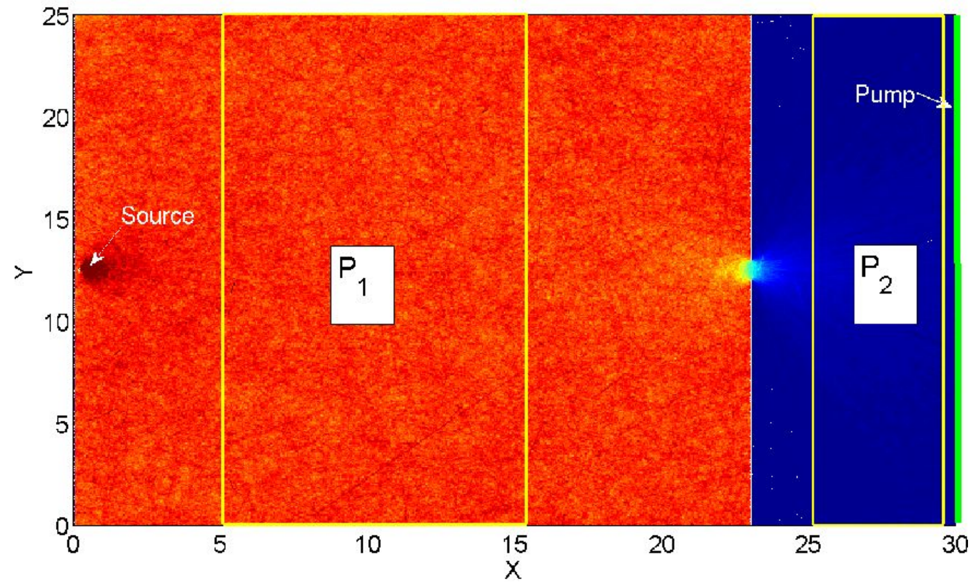
- Complex 3D geometry (divertor, bypasses etc...) can be handled.

- Can take into account collisions with wall, ionization, dissociation, charge-exchange, elastic collisions etc.

- In this benchmark purely diffusive b.c. and He gas are used .

Problem and set up





$$C = \frac{\frac{\partial N}{\partial t}}{n_1 - n_2}$$ conductance

$$\delta = \frac{p_1 L}{\mu v_0} = \frac{\sqrt{\pi}}{2k_n}$$ rarefaction parameter

- Aperture Geometries:
  - Slit and short channels
  - Orifice and short circular tube

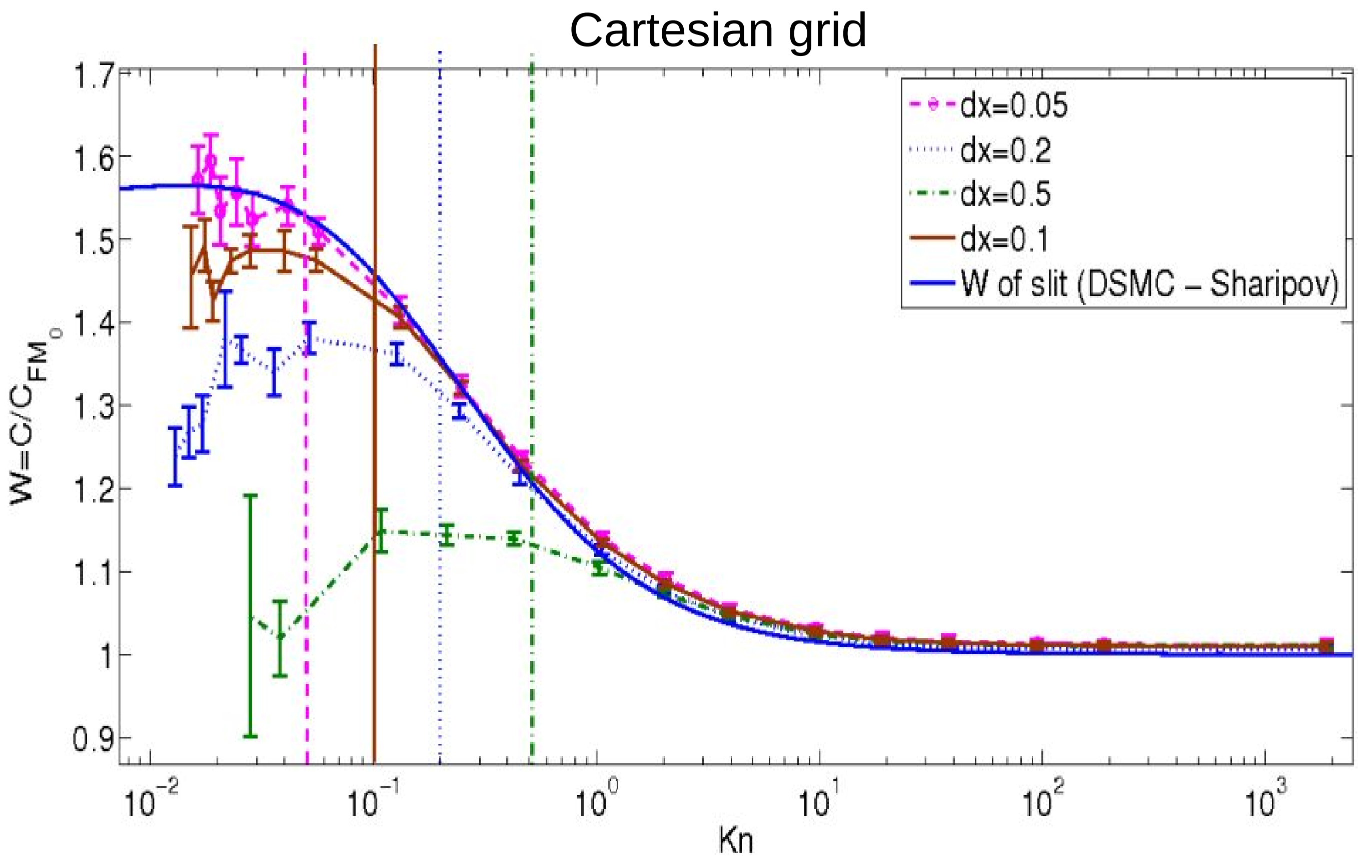
Choosing the grid

- For

$$k_n < \frac{\Delta x}{\lambda_{mfp}}$$

meanfreepath
< cell-size

=> gradients can not be resolved
⇒unphysical solution



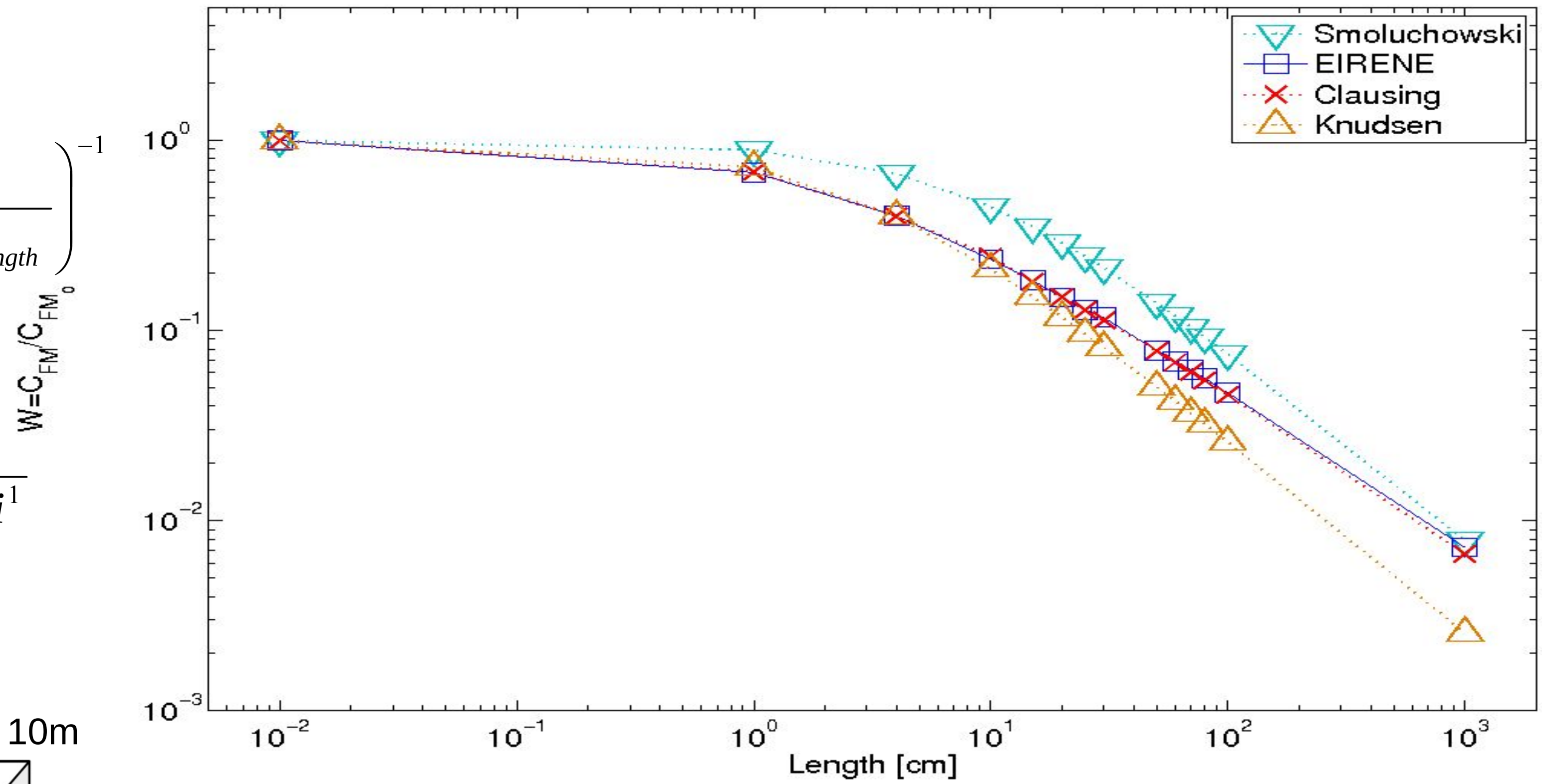
In this work grid limits to k_n>0.02, δ<40-50

Channel length scan in FMR

$$C_{FM} = \left(\frac{1}{1/C_{FM,0} + 1/C_{\infty-length}} \right)^{-1}$$

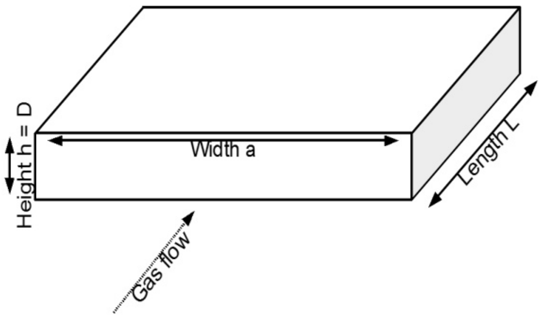
$$C_{FM,0} = \frac{1}{4} n v_a$$

$$C_{\infty-length} = \begin{cases} Knudsen^{1} \\ Smoluchowski^{1} \end{cases}$$



Height h=1cm

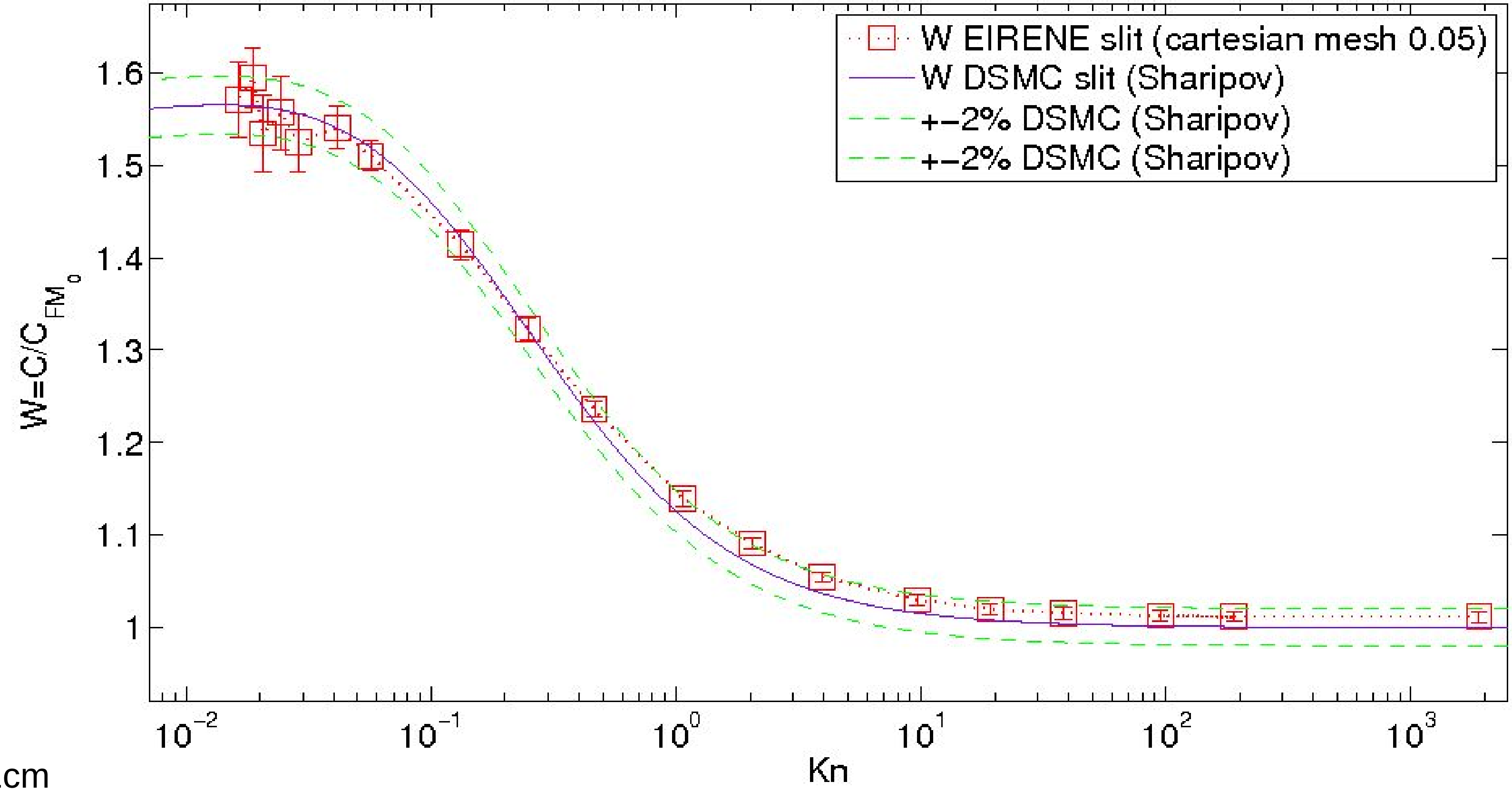
Reservoir volume= 1m x 1m x 10m



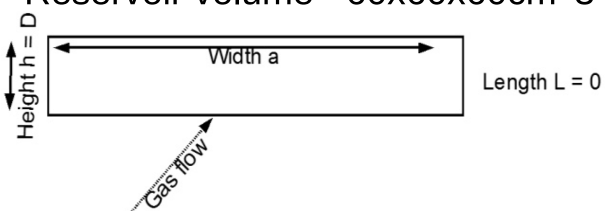
- Agreement within 0.3%, limited by statistic only

[1] J.M. Lafferty. Foundations of Vacuum Science. John Wiley and Sons, Inc., 1998

Slit case



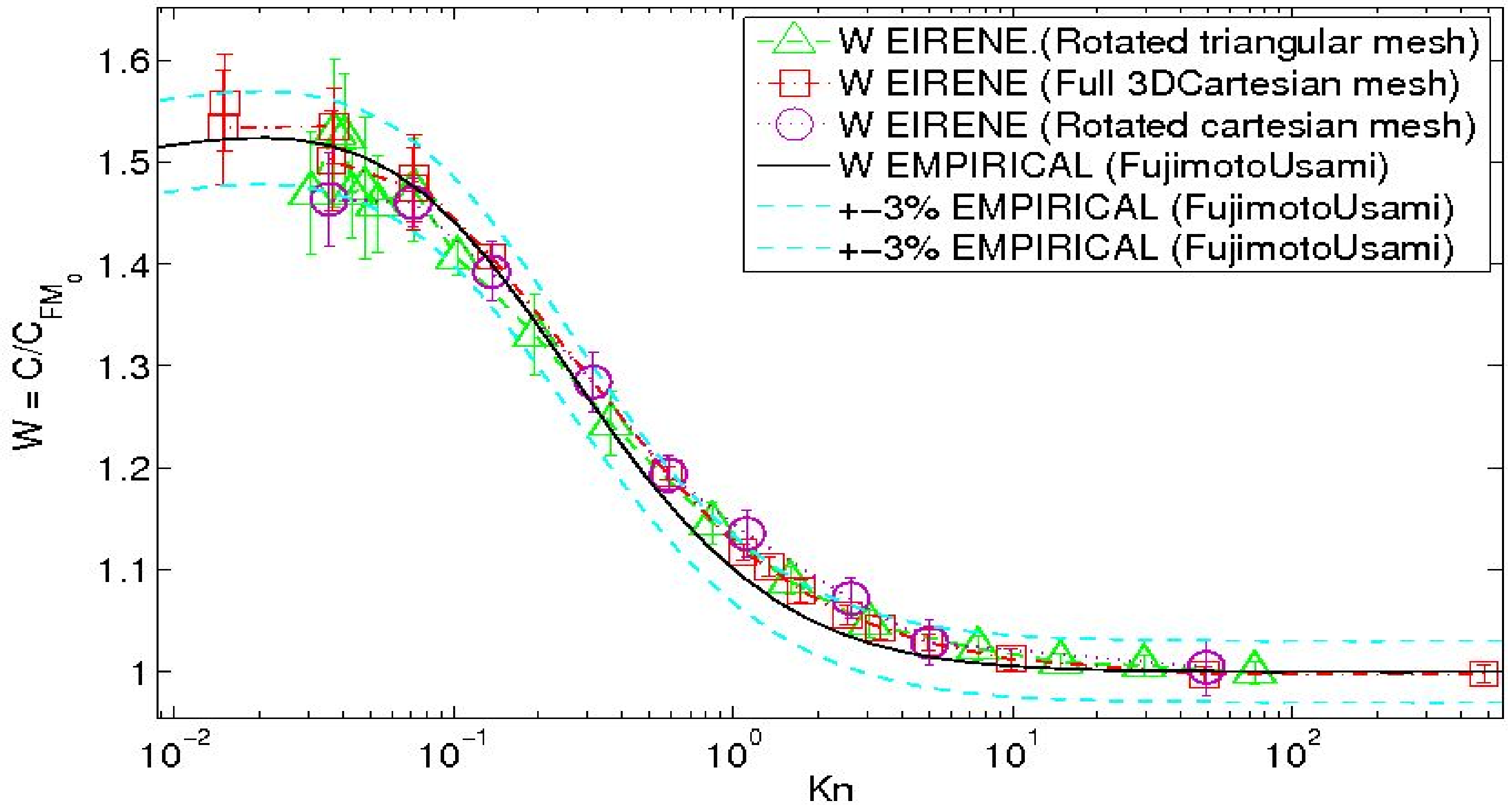
Height h=1cm
Reservoir volume =60x60x60cm^3



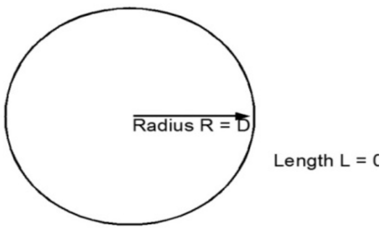
- Overall agreement with DSMC[1] simulations within 2%

[1] Felix Sharipov, Dalton V. Kozak. Rareed gas ow through a thin slit into vacuum simulated by the Monte Carlo method over the whole range of the Knudsen number. American Vacuum Society, 2009.

Orifice



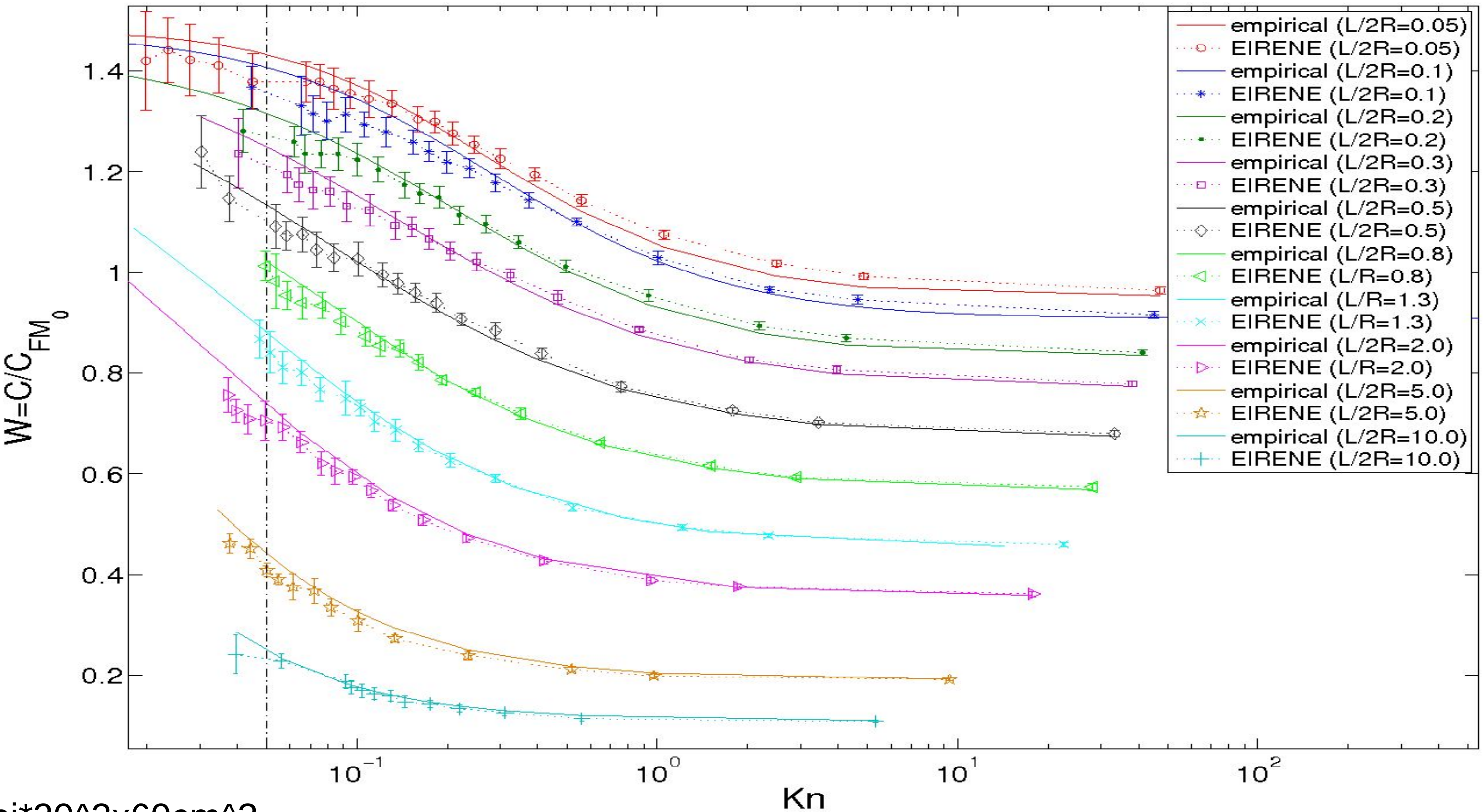
Radius R=0.5cm
Reservoir volume =pi*30^2x60cm^3



- Agreement with experimental data within 3%

Ref: T. Fujimoto, M. Usami. Rarefied Gas Flow Through a Circular Orice and Short Tubes. Journal of Fluids Engineering, 106, 1984.

Short pipes



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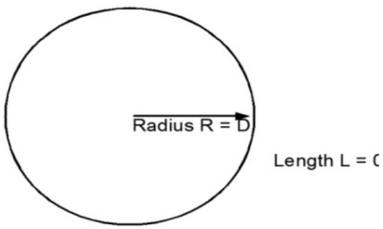
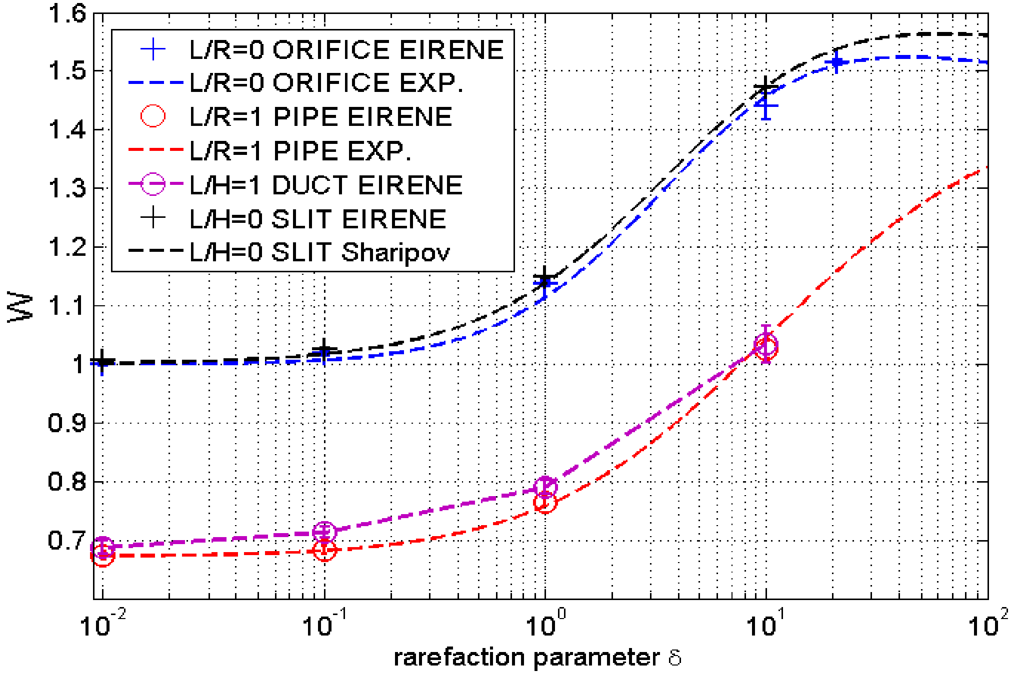


- Agreement with experimental data within 5%

Ref: T. Fujimoto, M. Usami. Rarefied Gas Flow Through a Circular Orice and Short Tubes. Journal of Fluids Engineering, 106, 1984.

Code performance



- Runs with higher statistic with parallelized version to check accuracy and performances
- Max. difference with DSMC is 3.5% for δ=10 in L/R=1 circular pipe

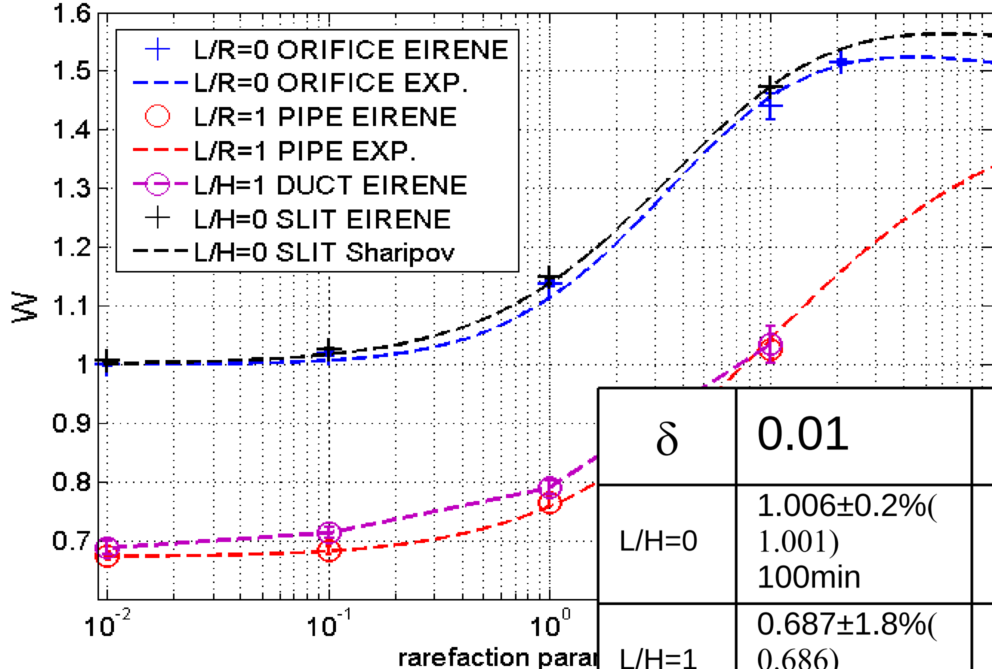
W EIRENE (Sharipov)
1 CPU time [s]

- δ=100 not clearly converged likely due to grid

Circular pipe

δ	0.01	0.1	1	10	100
L/R=0	1.000±0.4%(1.001) 60min	1.018±0.3% (1.014) 200min	1.138±0.4% (1.129) 730min	1.440±1.5% (1.462) 1000min	1.509±5.5% (1.534) >10000min
L/R=1	0.673±1% (0.673) 60min	0.683±1% (0.680) 160min	0.765±1% (0.754) 466	1.025±1.5% (1.062) 3000min	

Code performance



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Slit and short channel

δ	0.01	0.1	1	10	100
L/H=0	1.006±0.2%(1.001) 100min	1.026±0.2% (1.026) 200min	1.148±0.4% (1.148) 400min	1.472±1% (1.479) 4000min	
L/H=1	0.687±1.8%(0.686) 100min	0.713±1.3% (0.698) 300min	0.789±1.5% (0.767) 480min	1.034±3% (1.038) 2000min	

Circular pipe

δ	0.01	0.1	1	10	100
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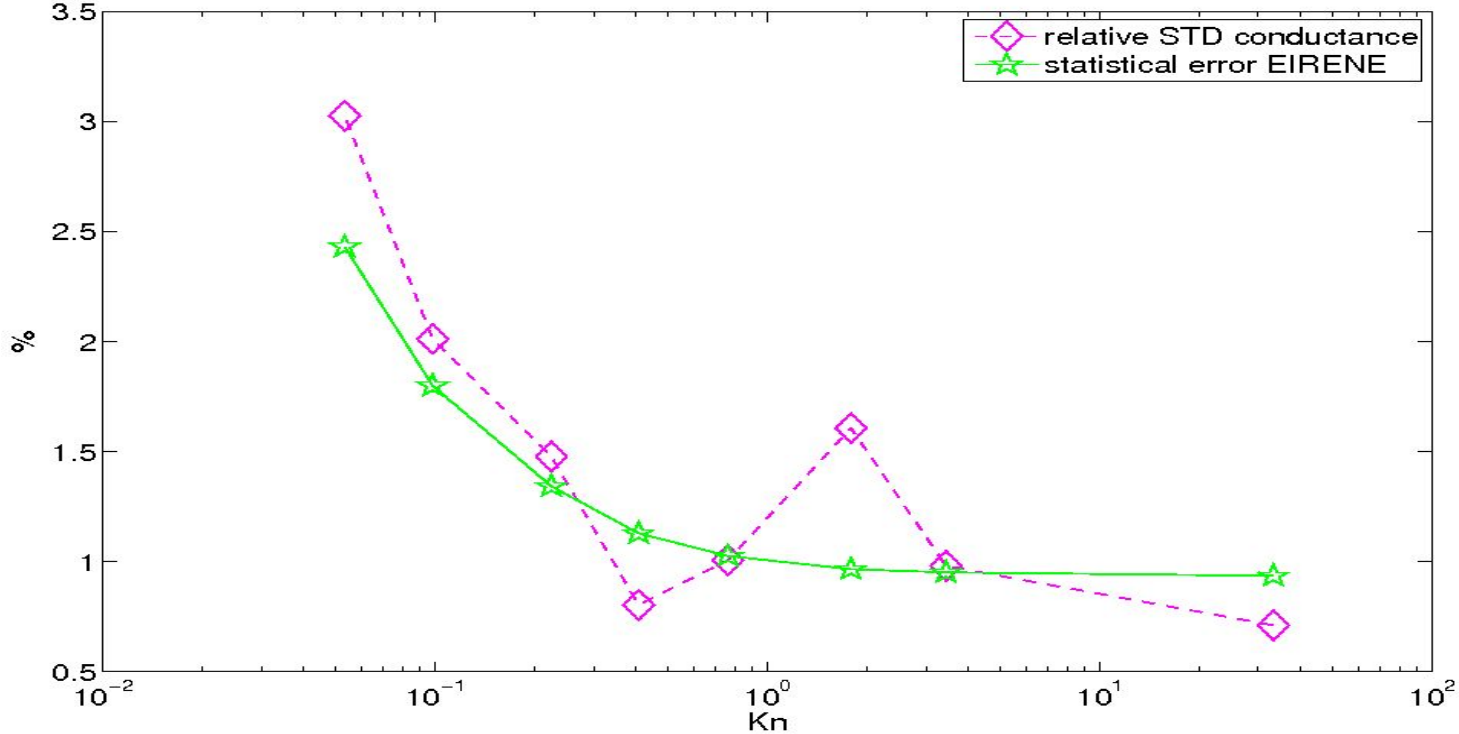
Conclusion and prospective

- Non-linear BGK agrees for δ<30 within 5% relative to DSMC and experiments
- Choice of the grid is crucial, no clear recipe yet
- Code not optimised for this task, but still it is very efficient for transition regime (about 8h for $\delta \sim 1$). And complex 3D geometry can be handled!

- Current development:
    - ➢ Use ES-BGK for correct P_r number
    - ➢ Optimise grids for δ up to 100
    - ➢ Understand better convergence properties

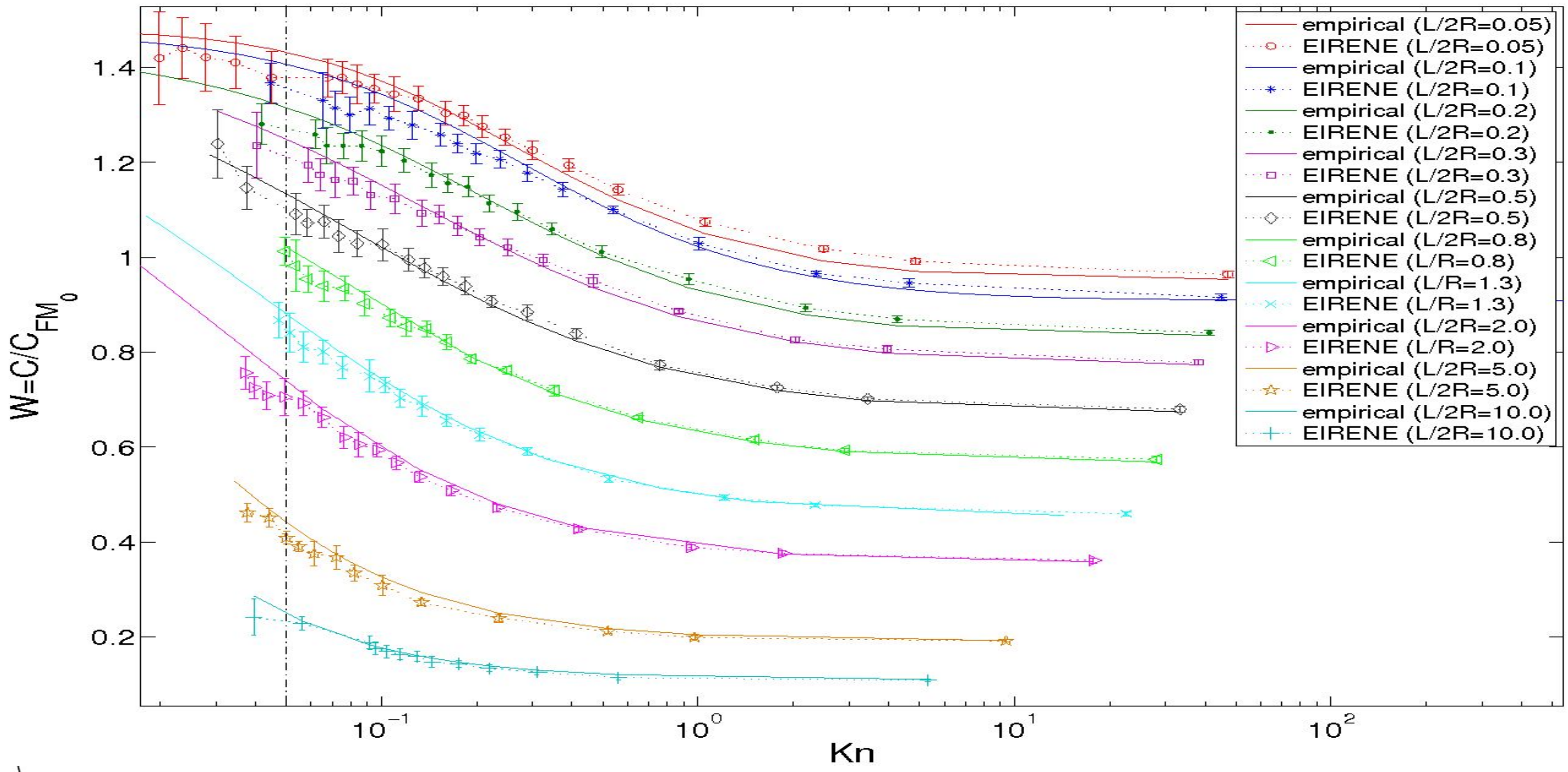
Back up slides

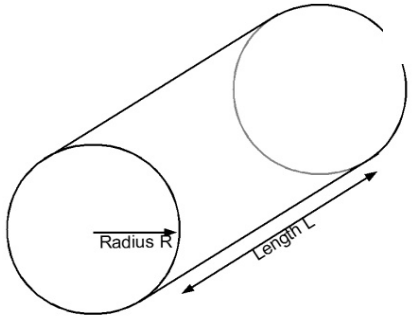
Statistical error



- STD of converged runs used as error estimator
- STD match statistical error resulting from Monte Carlo procedure

Pipes length scan



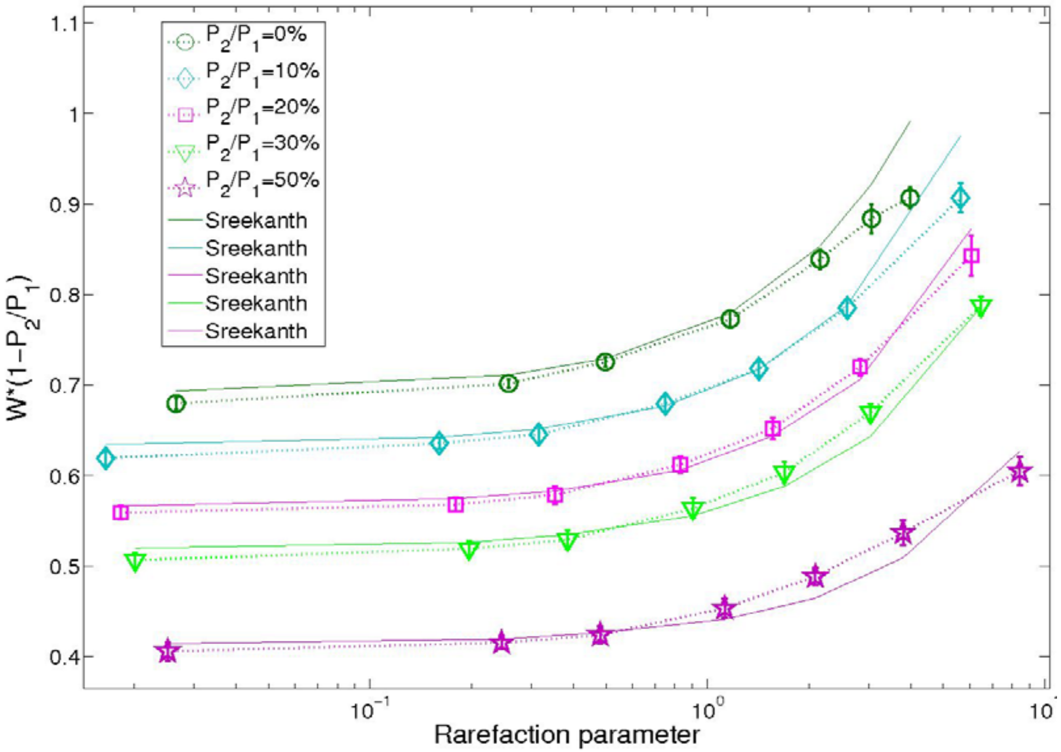


- Agreement within 5%

Ref: Tetsuo Fujimoto, Masaru Usami. Rareed Gas Flow Through a Circular Orice and Short Tubes. Journal of Fluids Engineering, 106, 1984.

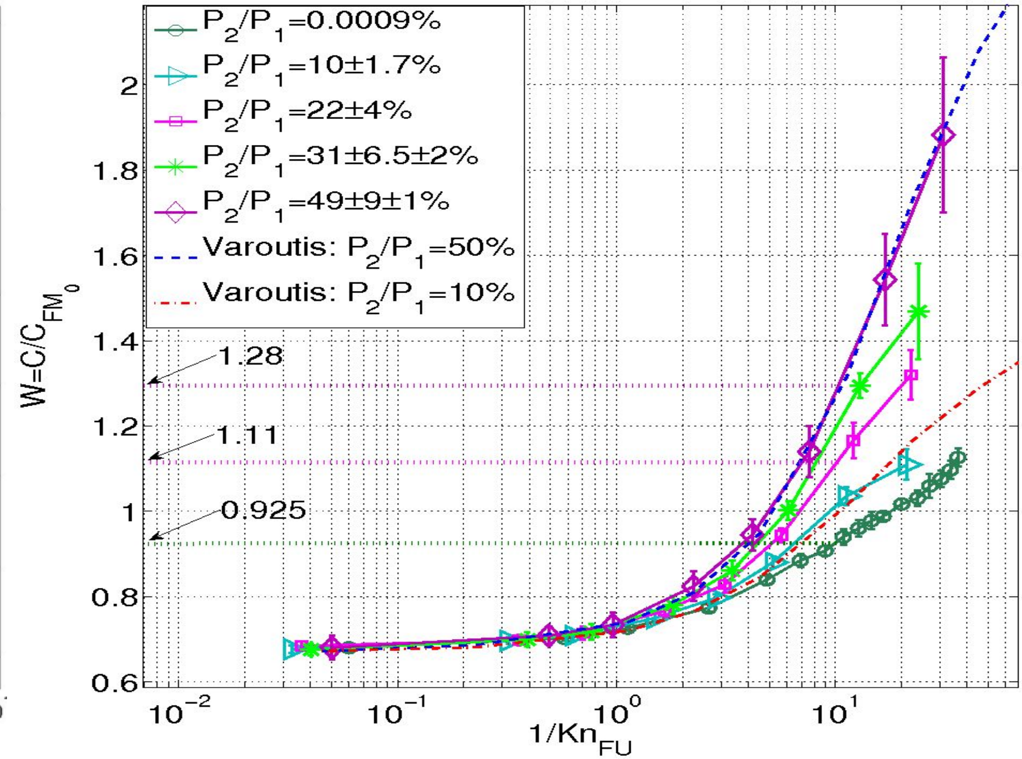
Pressure ratio scan

Circular tube with L/R=1



Ref: A.K.Sreekanth. Transition ow through short circular tubes. The Physics of
Fluids, 1965.

Circular tube with L/R=1

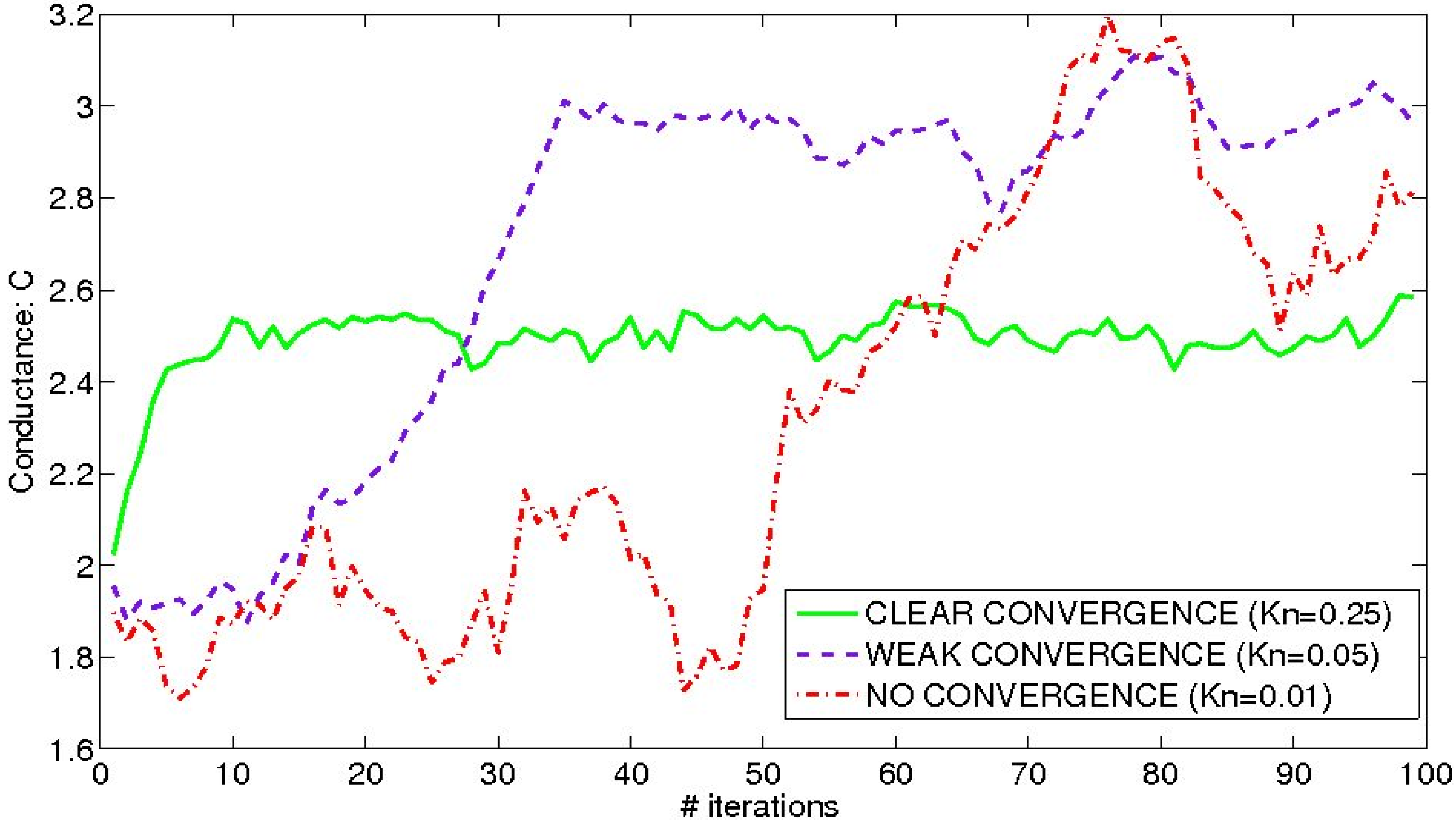


Ref: S.Varoutis, D.Valougeorgis, F.Sharipov. Simulation of gas flow through tubes of finite length over the whole range of rarefaction for various pressure drops ratios. Journal of Vacuum Science and Technology, 2009.

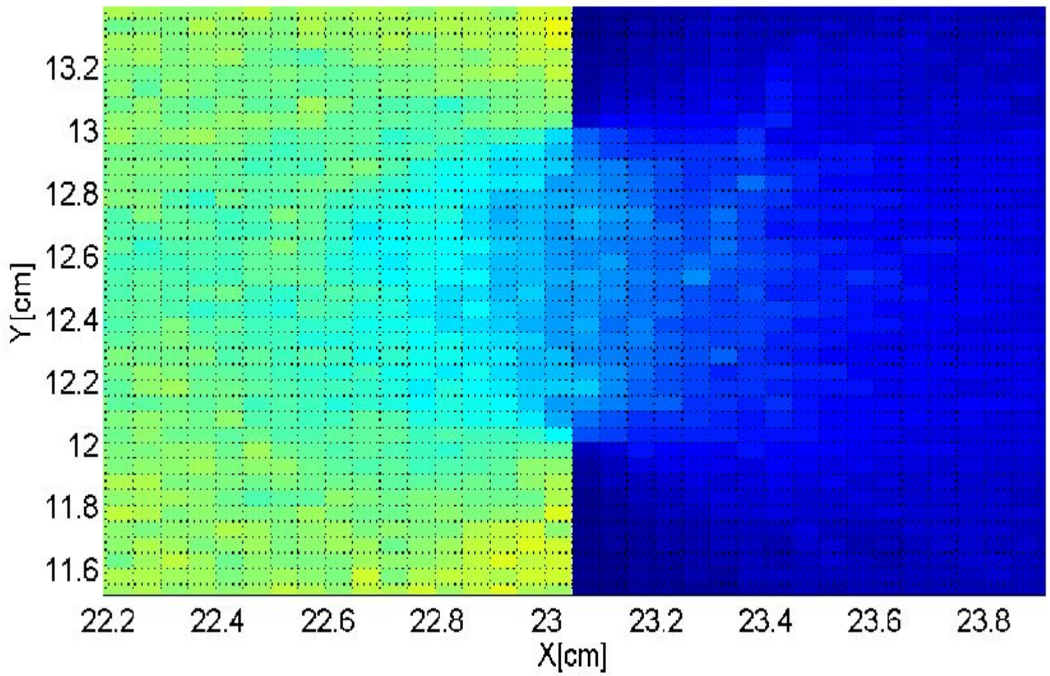
Agreement within 5% for Kn>0.1

Convergence

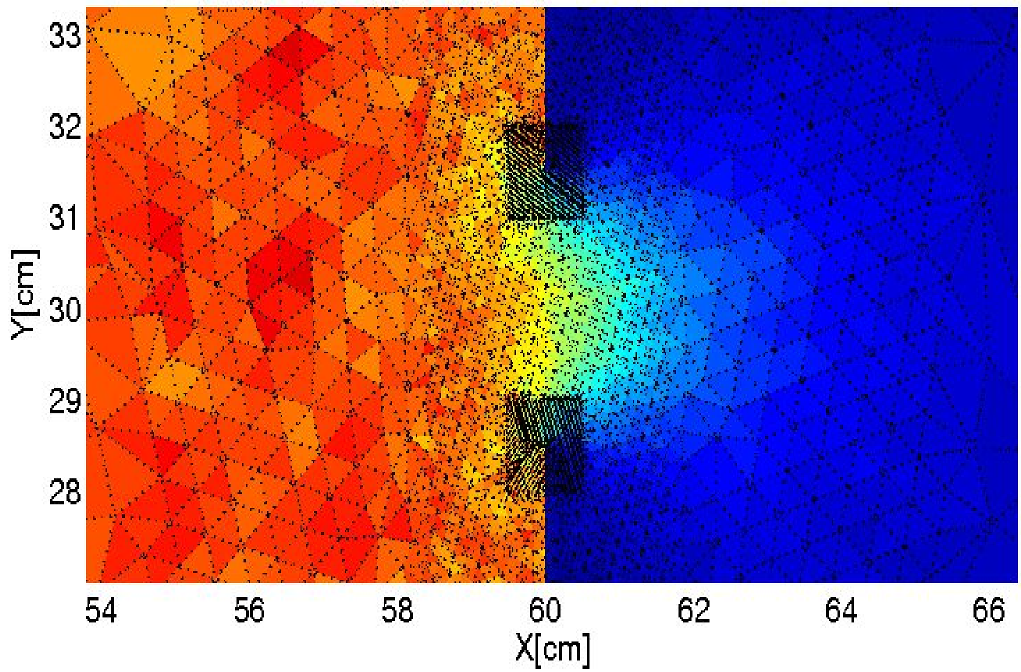
Convergence depends on grid resolution, statistics and Kn



Grids



Cartesian mesh

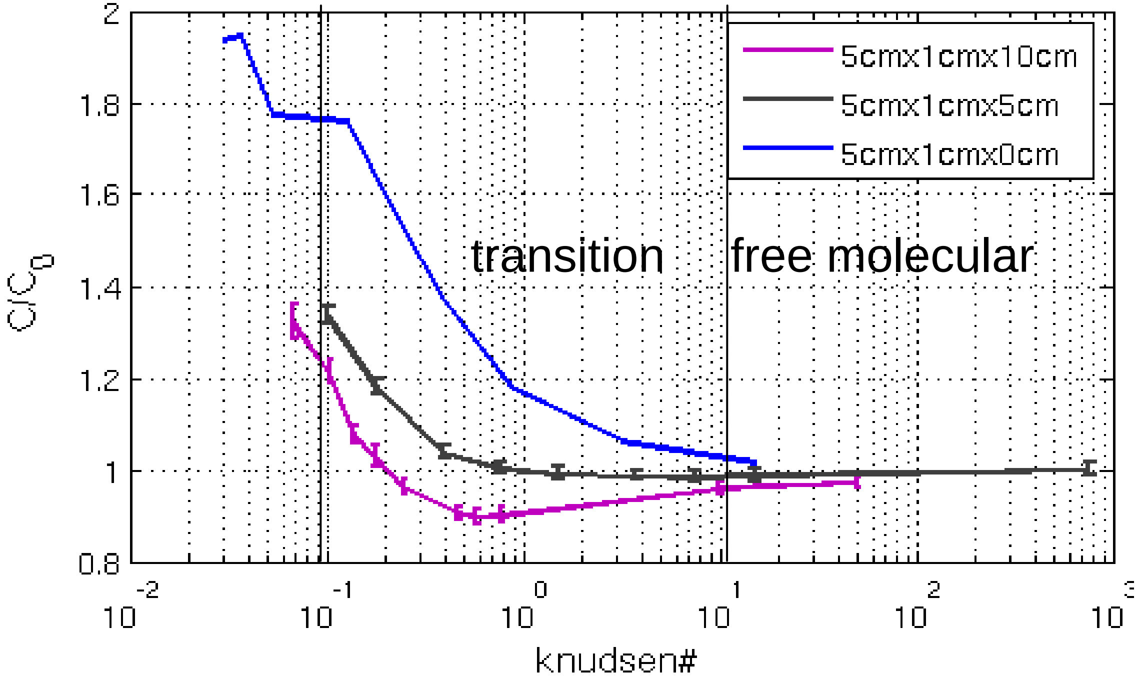


Triangular mesh

3D grids are generated by rotation or extension perpendicular to the plane

Expect behaviour of AUG conductances

Duct length scan L=0, 5 and 10 cm



- Qualitative trends are:
1. Long(short) duct/pipe (do not)show the Knudsen minimum
2. Strongly rectangular/elliptical duct show deeper minimum
3. Round/squared pipe/duct show “flat” behaviour near K_n =1.

- The conductance of AUG rectangular short ducts should be about 10% larger at K_n =1 and 40-80% larger at K_n =0.1
- Detailed calculation for AUG ducts geometry will be performed in the near future

$$\frac{df_i}{dt} = \sum_{j=i} \nu_{ij} \cdot \left(f_M^{ij} - f_i \right)$$

f^{ij}_M: shifted Maxwellian

ν_{ij}: velocity independent

$$n_{ij} = n_j, \quad \mathbf{u}_{ij} = \frac{m_i \mathbf{u}_i + m_j \mathbf{u}_j}{m_i + m_j}, \quad T_{ij} = T_i - \frac{2 \cdot m_i m_j}{\left(m_i + m_j\right)^2} \left[\left(T_i - T_j\right) - \frac{m_j}{6k} \left(\mathbf{u}_i - \mathbf{u}_j\right)^2 \right]$$